



# DIAMOND

Crystal and Molecular Structure Visualization

The screenshot displays the Diamond software interface. On the left, the 'Exploration Controller' window is open, showing a histogram of contact spheres around an oxygen atom. Below the histogram is a table of contact data:

| Atom 1 | Atom 2                     | d 1,2   | d-vdW      | Type         | File |
|--------|----------------------------|---------|------------|--------------|------|
| "O2"   | "C1"                       | 1.22245 | 1.197756   | Bond         |      |
| "O2"   | "H3" (-1+x, 1/2-y, -1/2+z) | 2.00797 | -0.623268  | A..H_inter   |      |
| "O2"   | "H1"                       | 2.34311 | -0.727886  | O..A_intra-2 |      |
| "O2"   | "C2"                       | 2.54472 | -0.875329  | Cnt_intra-2  |      |
| "O2"   | "H3A" (-1+x, y, z)         | 2.59816 | -0.0118426 | Cnt_inter    |      |
| "O2"   | "O3" (-1+x, 1/2-y, -1/2+z) | 2.81626 | -0.223743  | A..D_inter   |      |
| "O2"   | "H16B"                     | 2.91901 | 0.30901    | Cnt_intra-4  |      |
| "O2"   | "H8"                       | 2.95375 | 0.34375    | Cnt_intra-3  |      |
| "O2"   | "H21" (x, -y, 1-z)         | 2.97772 | 0.367723   | Cnt_inter    |      |
| "O2"   | "H7"                       | 3.03392 | 0.423919   | Cnt_intra-4  |      |
| "O2"   | "H19" (x, 1/2-y, -1/2-z)   | 3.12189 | 0.511895   | Cnt_intra-3  |      |
| "O2"   | "C16"                      | 3.14332 | -0.0766771 | Cnt_intra-3  |      |

On the right, a 3D ball-and-stick model of a molecular structure is shown. A tooltip for an oxygen atom is visible, displaying its coordinates and contact information:

```
"O2"
0.01781(15), 0.24607(9), 0.37314(11)
<< m_uiExploreFlags = 00000103 >>
Contact sphere with 1 H..A bond(s), 0 D..A contact(s), and 0 non-bonding contact(s)
Currently connected: 2 atom(s) [H1O1]
```

## New Version 5

The new Diamond version 5 contains several new features:

The most outstanding new feature is the **Exploration View**, which enables to study (strong) bonds as well as H-bonds and non-bonding contacts when checking for neighbouring atoms and molecules. A bond (or contact or H-bond, resp.) can be added or removed by clicking the checkmark in the distance table or shifting the boundary in the histogram or by clicking on the bond/contact in the structure picture graphics (see screenshot above).

The commands *Take Picture* and *Continue With New Picture* offer an improved workflow when creating multiple pictures for a structure data set.

The *More Pictures* docking window and the *Caption Bar* give a simplified overview of structure pictures.

Settings can be imported from version 4.

A newer version of Crystallography Open Database (COD; [www.crystallography.net](http://www.crystallography.net)) is available.

More outstanding functions:

- ✓ Import with automatic format recognition
- ✓ Build up structure pictures automatically or manually
- ✓ Schemes (style sheets) for building and design
- ✓ Structure type database
- ✓ Ellipsoids, disorder, mixed sites
- ✓ Molecules, packing diagrams
- ✓ Polymers and molecule clusters
- ✓ Fragmentated and broken-off bonds
- ✓ H-bonds and non-bonding contacts
- ✓ Preview of neighbouring atoms and -molecules
- ✓ Atomic environments from Dirichlet domains
- ✓ Coordination and Voronoi polyhedra
- ✓ Atom vectors, labels, and free text
- ✓ Reflection parameters and diffraction diagrams
- ✓ Distances, angles, and torsion angles
- ✓ hkl- and L.S.-planes and lines
- ✓ 3D export to POV-Ray, OBJ, and STL
- ✓ Video sequences and animations

Diamond version 5 will be/has been released in October 2023. The **update from Diamond 4 to 5 is free-of-charge**.

<https://www.crystalimpact.de/diamond/Default.htm>

| Price* for new License        | academic | regular |
|-------------------------------|----------|---------|
| Semiannual license (6 months) | 149,50 € | 299 €   |
| Annual license (12 months)    | 299 €    | 598 €   |
| Single license (permanent)    | 599 €    | 1.198 € |
| Site license (permanent)      | 1.198 €  | 2.396 € |
| Campus license (permanent)    | 2.396 €  | 4.792 € |

\* Prices do not include taxes which may be due.



**CRYSTAL IMPACT**  
H. Putz & K. Brandenburg GbR  
Kreuzherrenstr. 102  
D-53227 Bonn

Tel.: +49 (228) 981 36 43  
Fax: +49 (228) 981 36 44  
E-Mail: [info@crystalimpact.de](mailto:info@crystalimpact.de)  
<https://www.crystalimpact.de>